

## **REMARKS**

Claims 51-72 are pending in the above-identified application, claims 1-50 having previously been cancelled. Claims 51-72 stand rejected under 35 U.S.C. §112, and §102(b). With this Response, claims 51, 53, 54, 62-65, and 69-72 have been amended. Applicants traverse all rejections and respectfully request reconsideration of the claims in light of the remarks and amendments made in this Response.

Applicant thanks the Examiner and her supervisor for the courtesy of an Interview on November 30, 2004 with Jonathan Brecher and Leonid Thenor. Applicant has reviewed the Interview Summary and have no comments at this time.

### **I. Applicants' Invention**

The present invention relates to a method for use in deriving chemical structural information. The method includes the steps of dividing a chemical name into a series of fragments, associating the fragments with at least one data object known as a nomToken, and consolidating the list of nomTokens into a smaller list.

### **II. Claim Amendments**

Claims 51, 53, 54, 62-65, and 69-72 are amended. No new matter has been added with these amendments. Support for the claims can be found throughout the application, in particular at the following locations: page 13, line 19-page 14, line 5; page 14, lines 11-12; page 17, lines 11-13; page 19, line 20 - page 20, line 3; and page 18, lines 8-10.

### **III. Rejection of Claims Under 35 U.S.C. 112 – Written Description**

Claims 51-72 stand rejected under 35 U.S.C. 112 as allegedly containing new matter. The Office Action states that there is no basis in the specification for the generic method steps defined by new claims 51-72. Applicant respectfully disagrees.

Independent claim 51 describes a method of (1) acquiring a chemical name; (2) dividing the name; (3) associating each resulting fragment with a nomToken; (4) consolidating the list of nomTokens; and (5) repeating the consolidation step until only one nomToken remains. Independent claim 62 describes computer software that

comprises a set of instructions that perform the foregoing steps. Applicant submits that the originally filed claims, figures and description all support these claims.

The steps of claim 51 are described throughout the written description of the application. Applicant submits that, when read as a whole, the specification lays out the method of claims 51-72 in a section-by-section format. Each section of the specification describes a step of the method. For example, the step of acquiring a chemical name is described at page 4, lines 17-29. After acquiring the name, the specification presents an optional step of preprocessing the name at page 5, line 13 through page 13, line 14. Then, the step of dividing the name is described at page 13, lines 14-21. The sequential nature of the description is clear from the opening line of the description of the “dividing” step: “Once preprocessed, the name is divided into a series of fragments....” Page 13, lines 14-15.

After dividing the name into fragments, the step of associating each fragment with a nomToken is described at page 14, line 1 through page 18, line 8. The introduction to this section is clear to the reader: “Each known text string is associated in the lexicon with at least one data object known as a nomToken.” Page 14, lines 1-2. The following text of this section provides further support for this step, explaining the features of the nomToken and providing examples.

The next step of the method – consolidating the list of nomTokens – is described at page 19, line 19 through page 23, line 5. The first sentence of this section describes the generic method step: “A consolidation process derives, from a list of nomTokens, a smaller list that contains fewer nomTokens, *e.g.*, one nomToken.” Page 19, lines 19-20. The remainder of this section of the specification goes on to provide support for the consolidation step.

Finally, the repeating step of the method is described at page 23, line 6 through page 24, line 18. As with the other steps, it is clear from the text that this step is one of a series of steps described throughout the specification: “In the last stages of the consolidation process, multiple large groups are joined, so that typically, for example, ligands are joined to root structures, cations to anions, and esters to acids.” Page 23, lines

15-17. “[E]ach action following the fragmentation of the original input name has attempted to reduce the number of nomTokens in the resulting list. If the list has been reduced by this point to a single nomToken, the nomToken’s connection table, if present, represents the structure corresponding to the original input name.” Page 24, lines 9-13. As with the other sections of the specification, the remainder of this section provides support for this step of the method.

Similarly, independent claims 54 and 65 are also described throughout the written description of the specification. Each of these steps are easily identified by reading the written description as a series of steps, some more particular than others, for parsing a chemical name and deriving a chemical structure. These claims describe a method and computer software, respectively, that include the steps of (1) acquiring a name; (2) dividing the name; (3) associating each text string with a nomToken; (4) examining the nomTokens for a series of environments; (5) modifying the nomTokens; and (6) repeating the examining and modifying steps. As described previously, the first two steps of acquiring a name and dividing it are described at page 4, lines 17-29 and page 13, lines 14-21. Support for the step of associating each fragment with a nomToken, wherein each nomToken has particular features is described beginning at page 14, line 21, with the description of the features being described at page 14, line 21 through page 15, line 2. Pages 15-17 then provide definitions and illustrative examples of each of the features. The examining step and the modifying step are described at page 21, line 4 through page 22, line 4. This section explains that the process “begins with environments that are most specific” (page 21, lines 4-5) and then “continues with a series of less-localized nomenclature types...” (page 21, line 14). This section further explains how the nomTokens are modified when an appropriate environment is identified.

The Office Action further states that certain steps have been omitted in the generic steps of the pending claims. Applicant disagrees and submits that nowhere in the specification, figures or originally filed claims were any steps disclosed as being essential. The figures and the as-filed claims clearly indicate an intention to claim a generic method. For example, Figure 2 provides a flow diagram of a generic method of parsing a chemical name to derive a chemical structure. As noted at page 4, line 17

through page 5, line 4, Figure 2 is an embodiment of the present invention. Figures 3A and 3B describe another embodiment of the present invention, which includes additional steps for deriving chemical structures. The specification is organized by following the steps of Figures 3A and 3B. Page 5, lines 11-13. However, nowhere in the specification are any of these steps described as essential. Rather, by comparing the disclosure of the embodiment of Figure 2 and the disclosure of the embodiment of Figure 3, it is clear that the inventor also contemplated embodiments varying in scope between these two examples. Moreover, the specification states, "Other embodiments are within the scope of the following claims." Page 29, lines 17-18.

In addition, Applicant submits that the originally filed claims contemplated generic methods that also did not include all the specific processing steps described in the specification. Originally filed claim 1 recited:

A method for use in deriving chemical structural information, comprising:  
parsing a chemical name into at least first and second fragments; and  
determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second diagrammatic representations of the first and second fragments.

Originally cited claim 2 recited:

The method of claim 1, further comprising: identifying, among a preselected set of text strings, respective first and second text strings that correspond to the first and second fragments; and basing the determination of the first and second diagrammatic representations at least in part on conditions associated with the first and second text strings.

As seen from the text of the originally filed claims, the inventor contemplated a generic method of deriving chemical structural information.

As previously stated, there is no language in the specification that contemplates that specific processing steps are essential to the invention. Rather, the specification provides

various steps that can be included in various embodiments of the present invention, all within the scope of the generic methods of the originally filed disclosure. Accordingly, Applicant submits that the generic steps of the claimed invention are fully supported by the original disclosure.

Applicant submits that these remarks render the new matter rejection under 35 U.S.C. 112 moot. Therefore, Applicant requests that this rejection be withdrawn.

#### **IV. Rejection of Claims Under 35 U.S.C. 112 – Enablement**

Claims 51-72 stand rejected under 35 U.S.C. 112 as allegedly being non-enabled. Applicant respectfully traverses.

The Office Action states that the amended claims omit critical steps to achieve the desired result. Applicant disagrees. As explained above, nowhere in the specification are any steps characterized as “critical”. Specifically with respect to the preprocessing step mentioned in the Office Action, this step is omitted from Figure 2, which is an embodiment of the invention. Moreover, this step was not included in either original claim 1 or 2, both of which are embodiments of the invention.

The Office Action also states that the terms “locant map,” “attach-in map,” and “attach-out map” are not enabled. Applicant disagrees. Each of these terms is described in detail at pages 15-16. For example, “locant map” is defined at page 15, lines 4-5: “The locant map associates names of individual atoms with respective specific locations in the connection table.” Similarly, “attach-in map” and “attach-out map” are defined at page 15, lines 10-14: “The attach-in map functions similarly to the locant map and stores a list of atoms identified in the connection table that are considered to be awaiting attachment. ... The attach-out map associates a specific bond order to an attachment.” Further explanation of these terms is provided in the text following the definitions. Moreover, an explanation of how the attach-out map feature functions is provided in the description of Figure 7D (page 26, lines 5-10). Applicant submits that with these definitions and explanations, a person of skill in the art would understand the metes and bounds of these terms.

The Office Action further states that claim 53 is not enabled because the metes and bounds of the terms “examining the environment” and “compatible with the environment” are not defined. Applicant submits that amended claim 53 is enabled. The examination step of the consolidation process is described in detail at pages 19-20 of the specification. Applicant submits that, based on the guidelines provided in the specification a person of skill in the art would understand how to determine that an environment is compatible with a particular nomToken. For example, when a nomToken of type kTypePrefix, such as “pent”, is followed by a nomToken of kTypeYl, such as “yl”, a compatible environment is identified, *i.e.*, an alkyl chain. See page 21, line 16 through page 22, lines 1. The names are combined to form “pentyl”, an appropriate connection table is constructed, and a new nomToken is assigned, reflecting the combined string.

The Office Action states that claim 54 is not enabled. Applicant disagrees. In certain embodiments, the ranking provides a consistent order in which to consider each of several nomTokens in cases where a single text string fragment may be associated with multiple nomTokens. The generation of a ranked list of nomTokens is described first at page 17, lines 10-13. The Specification describes the creation of a parallel list of nomTokens, when a fragment of the chemical name is represented by more than one nomToken. The “nomToken having the highest-ranked type is chosen, at least initially.” Page 17, lines 12-13. Another use of the ranking system during the consolidation process is described at page 20, line 11 through page 21, line 13. Applicant submits that with these explanations, a person of skill in the art would understand how to generate a ranked list of nomTokens.

#### **V. Rejection of Claims Under 35 U.S.C. 112 ¶ 2**

Claims 51-72 stand rejected under 35 U.S.C. 112 as allegedly being indefinite. Applicant respectfully traverses. Nevertheless, solely in an effort to expedite prosecution, claim 51, 53, 54, 62 and 65 have been amended as described below to more particularly point out the claimed subject matter. Applicant submits that the claims are allowable as amended.

The Office Action stated that the claims were inconsistent with the Specification because the Specification indicated that the nomToken included the text of a known string, while the claims did not include the text as part of the nomToken. Claims 51, 54, 62, and 65 have been amended to state that the text string fragment comprises the name of each nomToken.

The Office Action stated that the phrase “to help cause” in claim 62 was confusing. Claims 62-65 and 69-72 have been amended to remove this phrase.

The Office Action stated that there was no antecedent basis for “the list” in claims 51 and 62. Claims 51 and 62 have been amended as follows: “associating each text string fragment with at least one data object known as a nomToken thereby creating a list of nomTokens.”

The Office Action further states that the phrase “uncommon character of chemical significance” is indefinite. Applicant disagrees. An example of such a character, “ $\mu$ ” is given at page 6, line 1. Applicant submits that, with this example, a person of skill in the art would understand the types of characters that are included in this phrase. For example, the “ $\pm$ ” character is an uncommon character of chemical significance. This character is described in the Appendix materials accompanying the original submission. As known to those of skill in the art, this character denotes the optical rotation of the chemical structure. However, because this is an uncommon character, it is spelled out as “plusminus.”

#### **VI. Rejection of Claims Under 35 U.S.C. 102(b)**

Claims 51-72 stand rejected under 35 U.S.C. 102(b) as allegedly being anticipated by U.S. Patent No. 5,345,516 (Boyer et al.). Applicant respectfully traverses.

Boyer et al. do not disclose generating chemical structural information based on a **chemical name**. Rather, all of the examples of Boyer et al. involve generation of chemical structures based on molecular formulae. The parsing steps of Boyer et al. are set forth in Appendix J. ‘516 patent, col. 11, lines 22-28. Seven definitions of chemical strings (S0-S6) that are processed by the invention of Boyer et al. are defined at columns

73-76. As shown in the examples provided to the right of each string definition, each of these string types involve molecular formulae (*e.g.*, CHCl<sub>2</sub>, C<sub>5</sub>H<sub>10</sub>). Unlike the examples provided throughout the instant application, none of these text strings contains a chemical name. Moreover, there is no teaching regarding the parsing of a chemical name. In contrast, the instant specification provides description of parsing chemical names and associating the text string fragments with nomTokens, which are then further analyzed to derive the chemical structure that is represented by the name.

For the foregoing reasons, Applicant submits that the claims of the instant application are not anticipated by Boyer et al.

## **VII. Conclusion**

In view of the foregoing remarks, Applicants submit that all pending claims are in condition for allowance, which action is earnestly solicited.

Applicants respectfully request an early and favorable reconsideration and issuance of this application as amended herein. The Examiner is encouraged to contact the undersigned to expedite prosecution of this application.

Applicants also include a petition for a two-month extension of time to extend the period for response up to and including January 11, 2005. An authorization to charge the associated fee of \$450.00 to our Deposit Account No. 08-0219 accompanies this response.

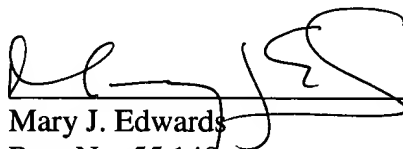


No other fees are believed to be due in connection with this submission.  
However, if any fees are due in connection with this application, please charge them to  
our Deposit Account No. 08-0219.

Respectfully submitted,

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